SUM-FREQUENCY GENERATION SPECTROMETER

DMR-0216904
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A sum-frequency generation (SFG) spectrometer purchased with NSF support is in operation at the University of Utah and is being used by researchers on campus and by external users to study the molecular structure of interfaces.

Sum-frequency generation

Sum-frequency generation is a second order nonlinear optical process forbidden in bulk media with inversion symmetry, but allowed at a surface or interface where the inversion symmetry is broken. Therefore SFG spectroscopy is highly surface specific. In SFG spectroscopy experiments two pulsed laser beams, one visible and the second infrared (IR), at frequencies ω_{vis} and ω_{IR}, overlap temporarily and spatially on an interface to generate an output at the sum frequency $\omega_{SF} = \omega_{IR} + \omega_{vis}$

Unique capabilities

i) recording vibrational spectra of nanoscale interfaces with no interference from the bulk
ii) determination of orientation, conformation and ordering of interfacial species at the molecular level

n

SFG Spectrometer Parameters

- **Spectral range:** 600 - 4300 cm^{-1} (IR wavelength: 2.3 - 18 μm)
- **Spectral resolution:** <6 cm^{-1}
- **In-depth resolution:** sub monolayer to thickness of interface
- **Lateral resolution:** *n* x100 μm
- **Sensitivity:** depends on interface structure, IR laser pulse energy, and probing laser beams polarization
- **Applications:** solid/solid, solid(liquid)/liquid, solid(liquid)/gas interfaces

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(continued)

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Recent advances in interface characterization by SFG

The liquid/air interfaces of alcohols and their mixtures with octyl hydroxamic acid (OXA) have been investigated. The SFG spectra support an all-trans alkyl chain conformation for the alcohols and a tilted chain close to the interface for OXA, Figure 1.

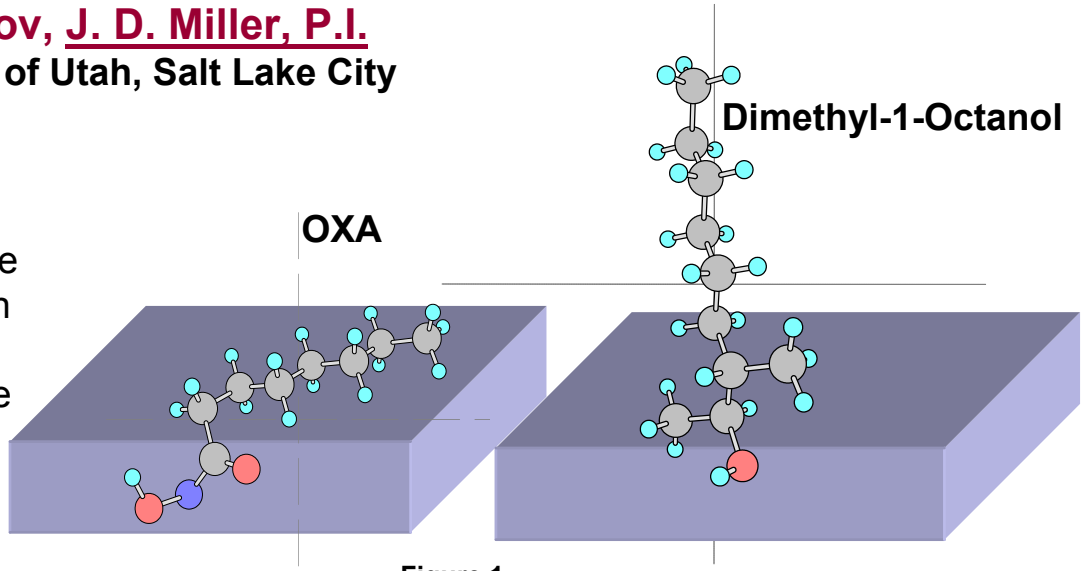

Figure 1

Mixed monolayers of a cationic lipid (dioctadecyldimethyl ammonium bromide - DOMA) and a neutral surfactant (stearic acid methyl ester - SME) have been studied at the water/air interface (Figure 2) and as LB films on mica. The mixed monolayers on water have their alkyl chains in close to all-trans conformation and with no gauche defects, in contrast to the pure lipid films, as seen in the CH stretching band region, Figure 2. The water structure below the mixed monolayers is well ordered and predominantly ice-like due to the interaction with the charged DOMA head groups and gives rise to a well-defined OH band.

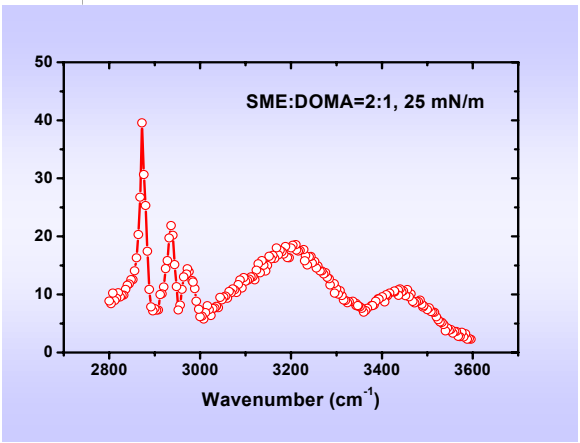

Figure 2
SFG spectrum of a mixed monolayer on water

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